Using Process Control Theory to Estimate Sea Spray Emissions in GEOS-Chem

Banff Workshop: Mathematical approaches of atmospheric constituents data assimilation and inverse modeling

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CAPD CENTER

CAPS Center for Atmospheric Particle Studies

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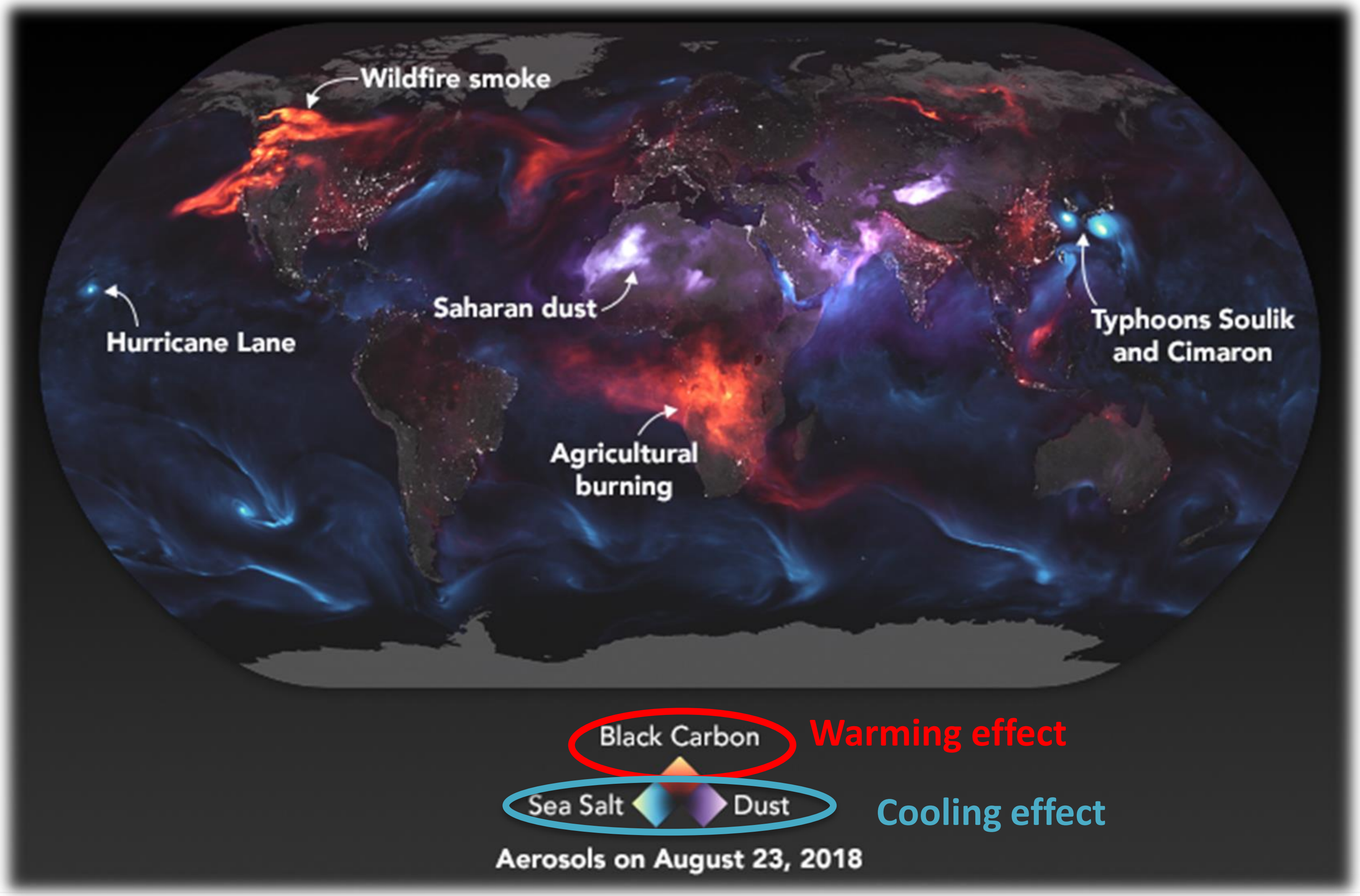
A day in the life of atmospheric aerosol
Sea spray generates sea salt aerosol



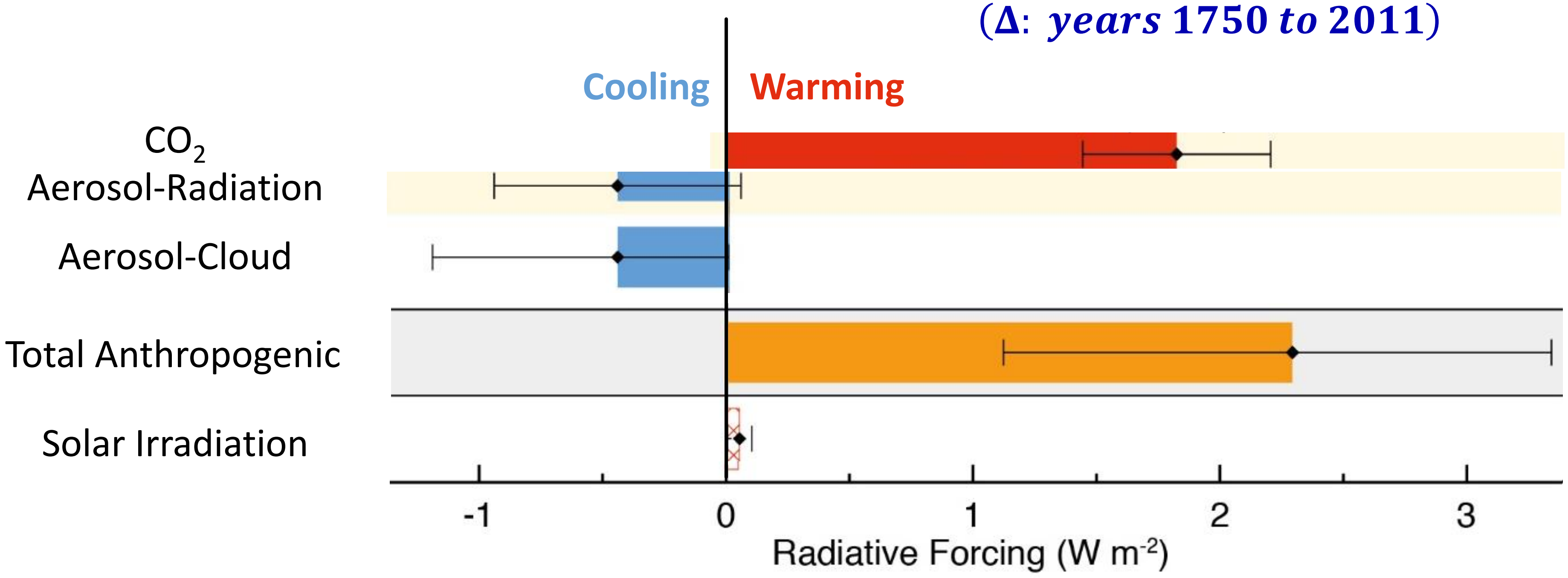
Joshua Stevens, using GEOS data from the Global Modeling and Assimilation Office at NASA's Goddard Space Flight Center. https://climate.nasa.gov/news/2793/just-another-day-on-aerosol-earth/

Improved atmospheric aerosol predictions lead to better predictions of climate change

The Intergovernmental Panel on Climate Change estimates radiative forcing to assess the effects of human activity on the climate.

$$\sim \frac{\partial E}{\partial c} \Delta c$$

$$(\Delta:\ years\ 1750\ to\ 2011)$$



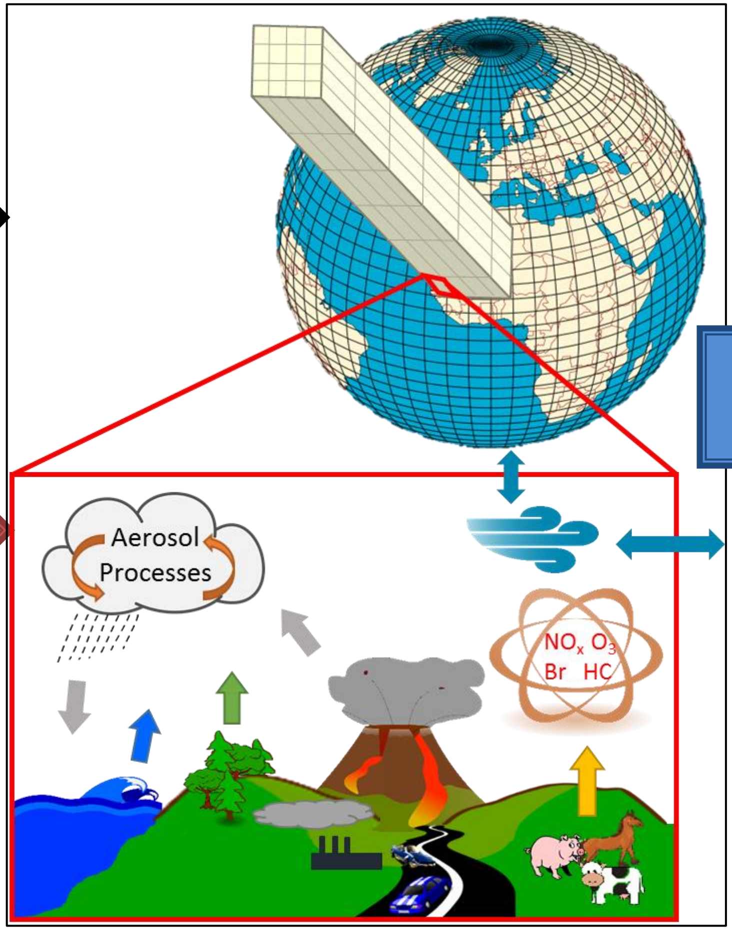
Anthropogenic and Natural Radiative Forcing. In: "Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change"

Chemical transport models predict gas and particle concentration fields

- GEOS-Chem is driven by NASA's MERRA2 meteorological reanalysis fields
- TwO-Moment Aerosol Sectional (TOMAS) algorithm used for aerosol processes
- Soot and organic carbon emissions from input data
- Dust and sea salt emission from parameterizations based on wind data
  - $E_{SSA}(D_p) \propto U_{10}^{3.41}$
  - Parameterization for sea spray from breaking waves based on field measurements on Hawaiian coast (Clarke, 2006)

Meteorology & Initial Conditions

Emission fields



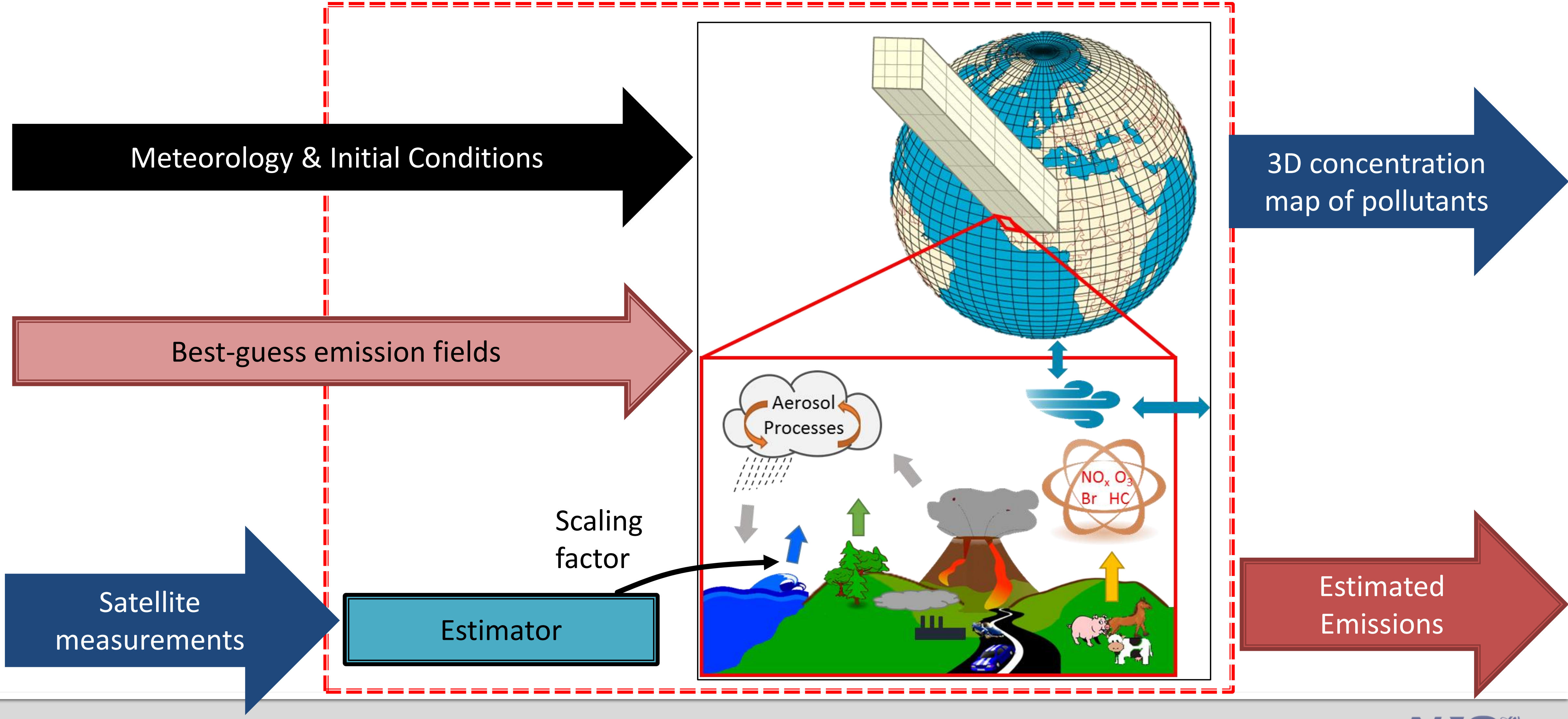
3D concentration map of pollutants

Clarke, A. D. et al. (2006) An ultrafine sea-salt flux from breaking waves: Implications for cloud condensation nuclei in the remote marine atmosphere. *Journal of Geophysical Research Atmospheres*

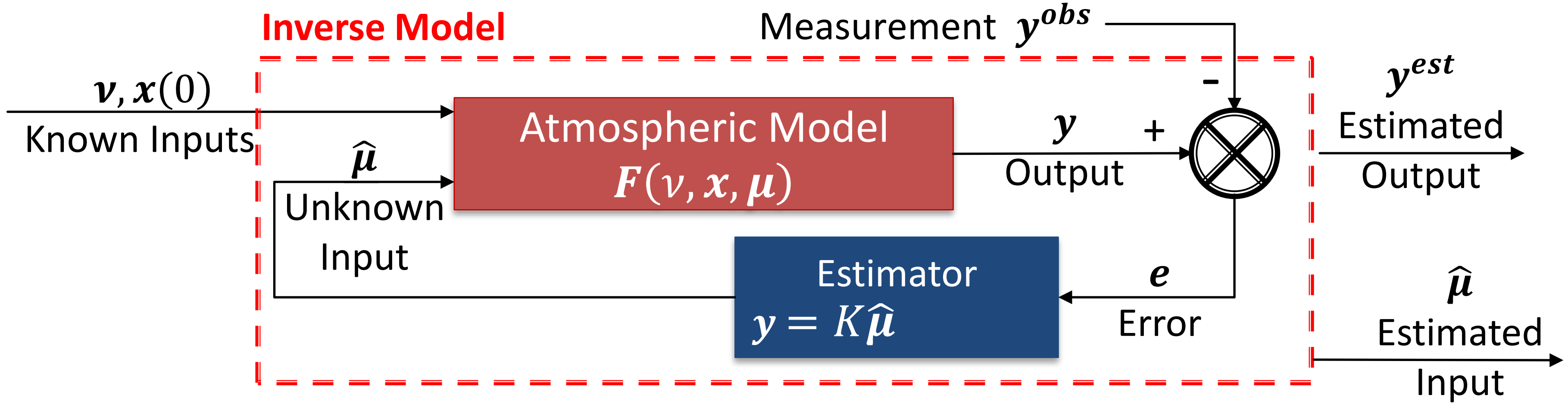
We can use satellites measurements of aerosol optical depth (AOD) to estimate aerosol emissions

Image courtesy of Levy, R., Hsu, C., et al., and the NASA Level-1 and Atmosphere Archive & Distribution System (LAADS) Distributed Active Archive Center (DAAC), Goddard Space Flight Center, Greenbelt, MD

Inverse modeling uses observations to estimate emissions



Process control can provide an improved atmospheric inverse modeling technique



Common methods based on least-square minimization:

- Kalman Filter: analytical solution (i.e. [1])
  - Requires reduced model or assumption of linear model: simplifications

[1] Prinn, R. & Hartley, D. *J. Geophys. Res.*, 98 (1993)
[2] Elbern, H & Hauke, S. *J. Geophys. Res.*, 104 (1999)
[3] Farschman, C. et al. *AIChE Journal*, 44 (1998)
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[5] Levant, A. *European Control Conference* (2001)

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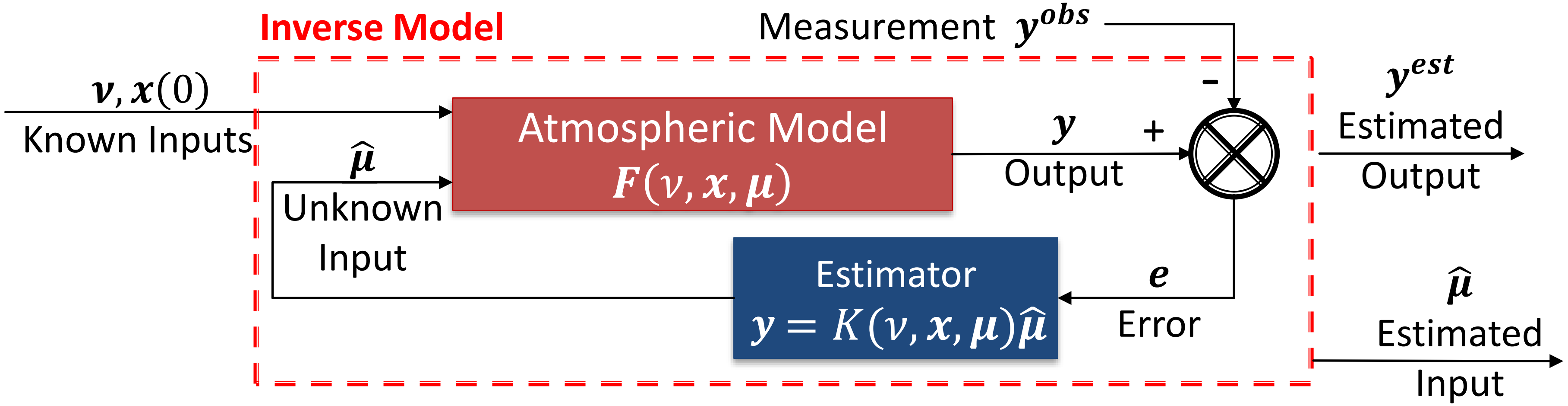

Common methods based on least-square minimization:

- Kalman Filter: analytical solution (i.e. [1])
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- "Adjoint method": numerically solve for Maximum A Posteriori (MAP) solution to inverse problem (i.e. [2])
  - ➢ Adjoint is a similar scale to atmospheric model: expensive
  - ➢ Calculation of model jacobian with adjoint model: obsolete after model updates

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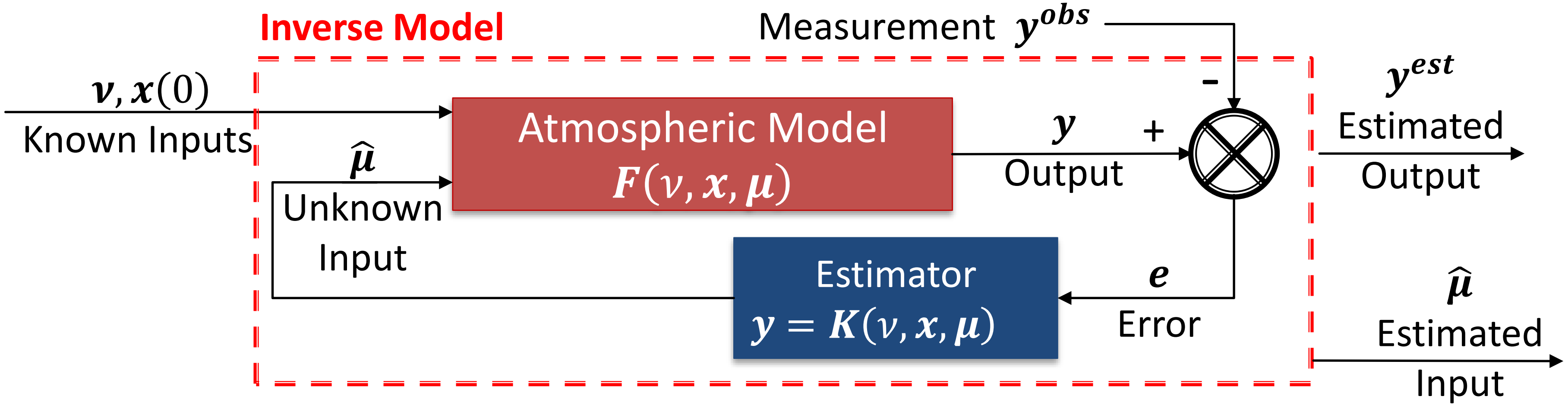

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This work formulates an input observer:

- Design an input observer based on passivity theory that estimates model inputs [3]
  - Need derivative of measurements; use available differentiation methods [4, 5]

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Passivity-Based Input Observer (PBIO) is based on dynamics of "inventory variables" (z)

$\boldsymbol{x}(\mathrm{t})$: concentration fields
$\boldsymbol{\nu}$: Known parameters
$\boldsymbol{\mu}(t)$: Unknown parameters

Dynamics of inventory variables ($\boldsymbol{z} \in \mathbb{R}^{N\times 1}$):

All other processes ($\mathbb{R}^{N\times 1}$)

Uncertain processes that we want to estimate ($N \times K$), i.e. $\boldsymbol{E_{SSA}}$

$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{f}(x, \nu, t) + G(\nu, t)\boldsymbol{\mu}(t)$$

Scaling factors applied to uncertain processes ($K \times 1$)

$$\boldsymbol{y_1}(t) = \boldsymbol{z}(t)$$
$$\boldsymbol{y_2}(t) = \dot{\boldsymbol{z}}(t)$$

The model error is defined as deviation between the estimated and measured inventory:

$$\boldsymbol{e}(t) = \boldsymbol{y_1}(t) - \boldsymbol{y_1^{obs}}(t) \qquad \frac{d\boldsymbol{e}}{dt} = \boldsymbol{y_2}(t) - \boldsymbol{y_2^{obs}}(t)$$

The goal is to find $\hat{\mu}$ that decreases the error, so we force the model error to exponentially decay.

$$\frac{d\boldsymbol{e}}{dt} = -K_c\boldsymbol{e}(t)$$

Tuning parameter $\in \mathbb{R}^{N\times N}$

$$K_{c_{i,i}} = \frac{1}{\tau_i}$$

Convergence timescale (hr)

Solve N×K system of linear equations!

$$\boldsymbol{f} + G\hat{\boldsymbol{\mu}}(t) - \boldsymbol{y_2^{obs}}(t) = -K_c\left(\boldsymbol{z^{est}}(t) - \boldsymbol{y_1^{obs}}(t)\right)$$

$$\Rightarrow \hat{\boldsymbol{\mu}}(t) = A^{-1}\boldsymbol{b}$$

Tatiraju, S. and Soroush, M., "Parameter Estimator Design with Application to a Chemical Reactor", *Ind. & Eng. Chem. Res., 37* (1998)
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$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{f}(x, \nu, t) + G(\nu, t)\boldsymbol{\mu}(t)$$

$$\boldsymbol{y}_1(t) = \boldsymbol{z}(t)$$

Scaling factors applied to uncertain processes ($K \times 1$)

Th

✓Computationally efficient & scalable

✓Does not simplify model equations

✓Independent of model updates

The

exp

Solve N×K system of linear equations!

$$\boldsymbol{f} + G\widehat{\boldsymbol{\mu}}(t) - \boldsymbol{y}_2^{obs}(t) = -K_c\left(\boldsymbol{z}^{est}(t) - \boldsymbol{y}_1^{obs}(t)\right)$$

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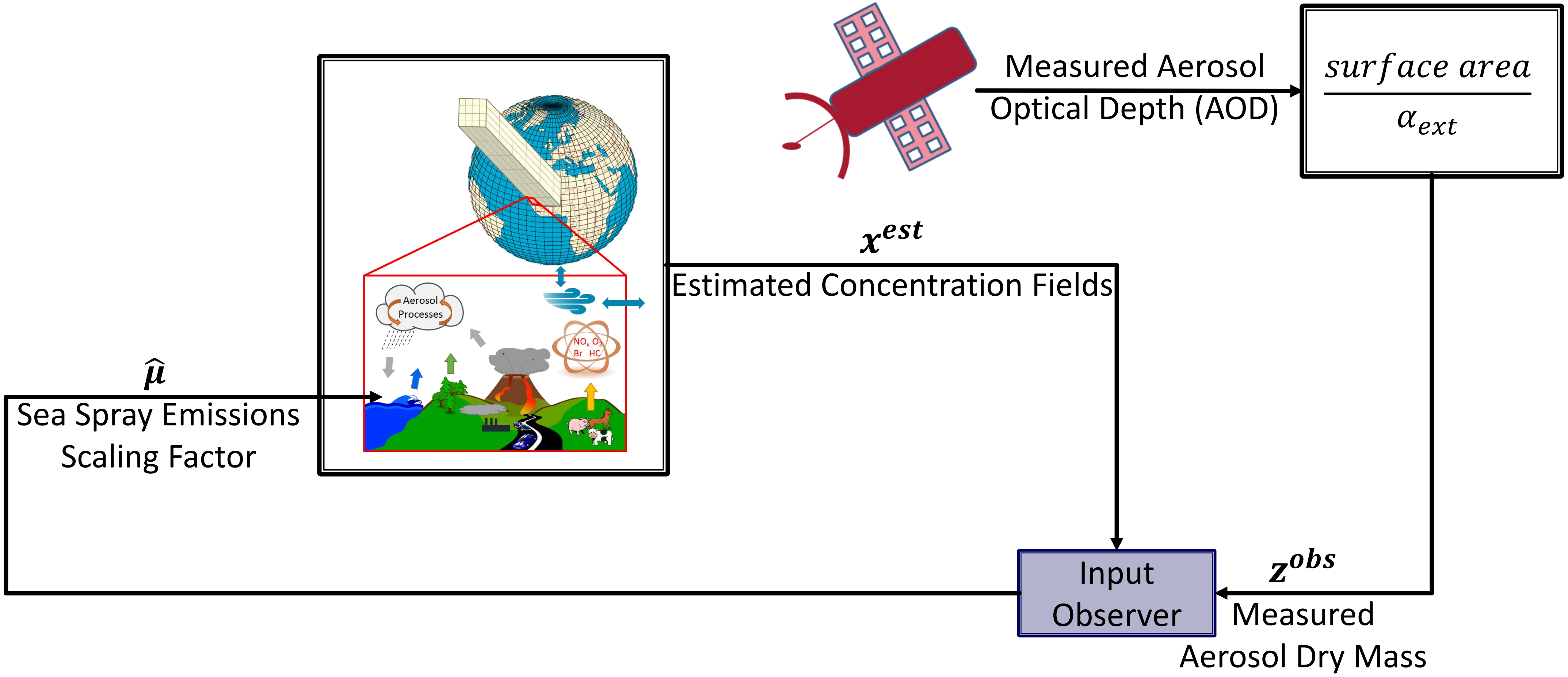
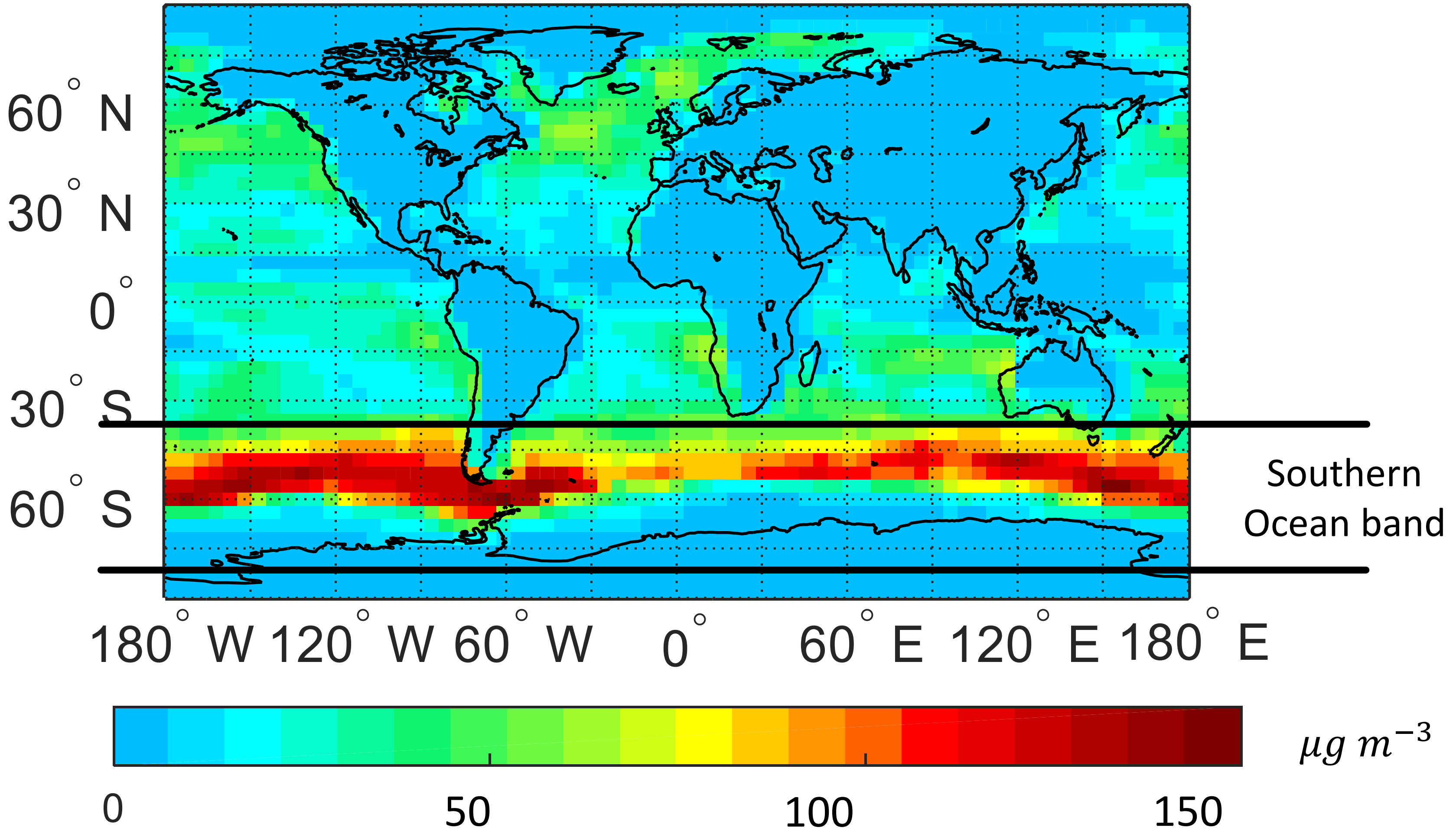
Use total aerosol mass inventory to estimate sea spray emissions with satellite data



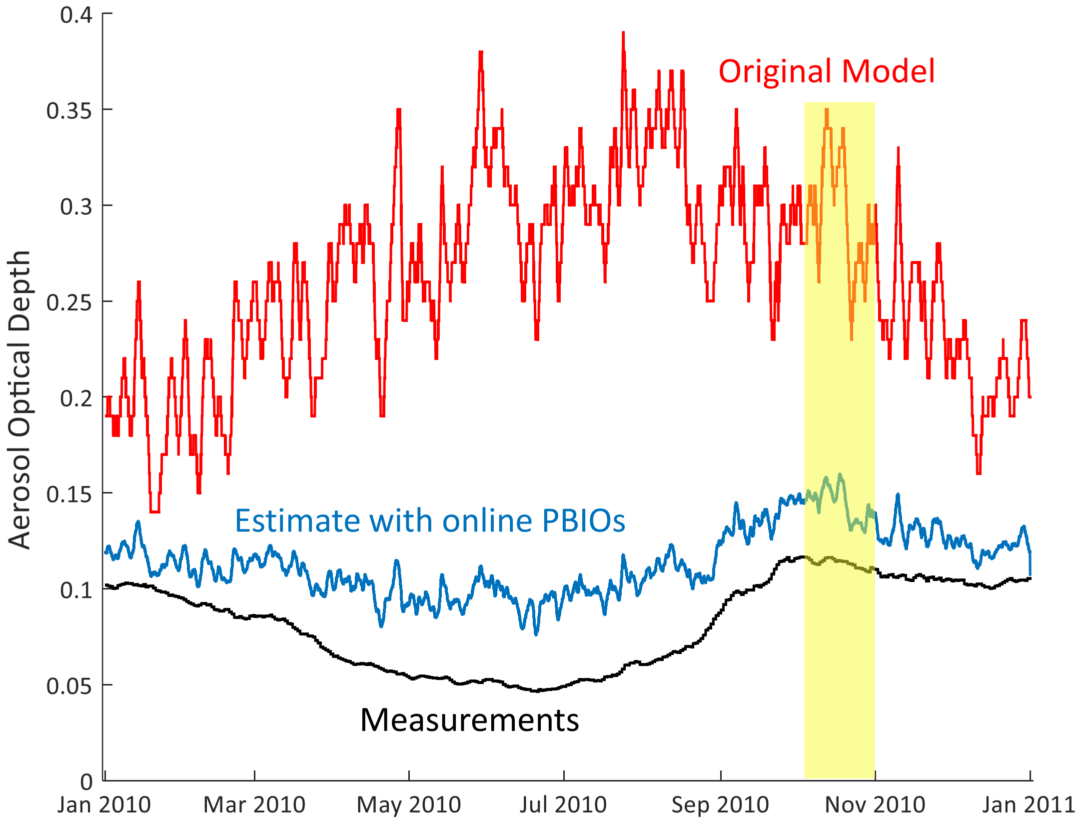
Global model over-predicts sea salt concentration over the Southern Ocean band

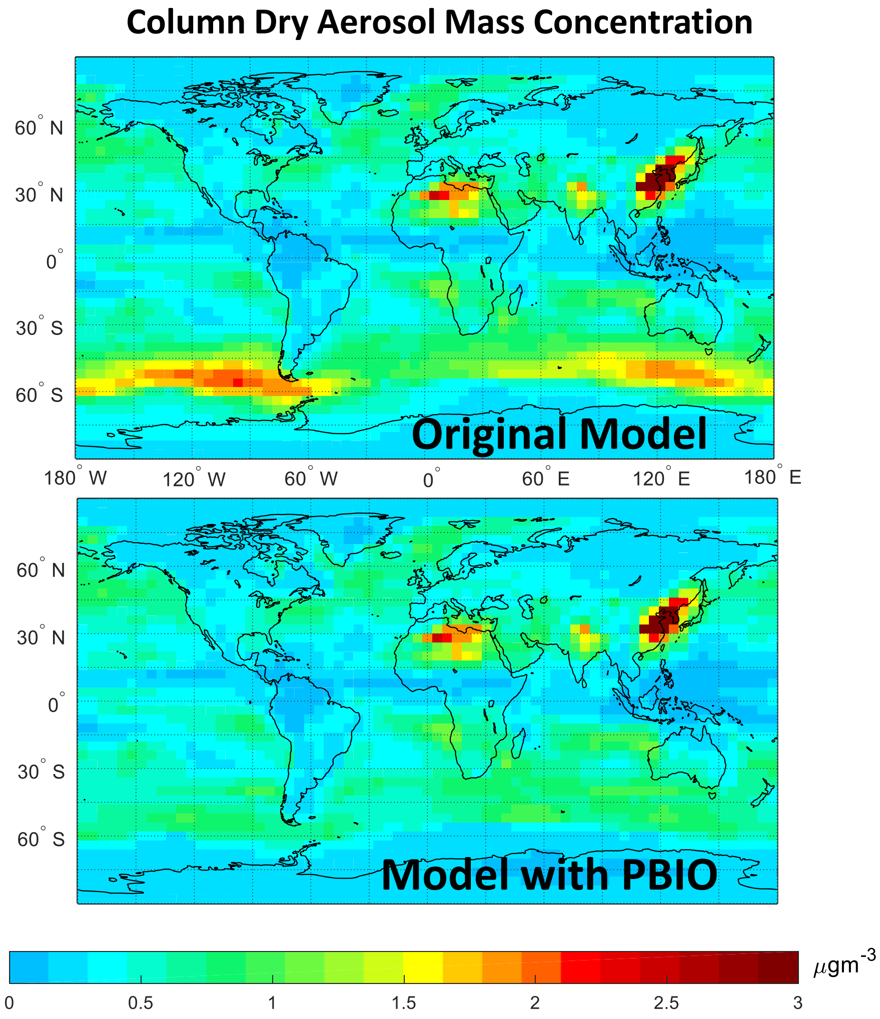
- October 2010: Surface NaCl aerosol concentration
- Predicted by GEOS-Chem TOMAS v9-02 at 4°x5° horizontal resolution
- Sea spray over-predicted in Southern Ocean due to high winds
- ➢ Use daily AOD measurements to scale sea salt emissions over Southern Ocean band



Model with online observers matches measurements

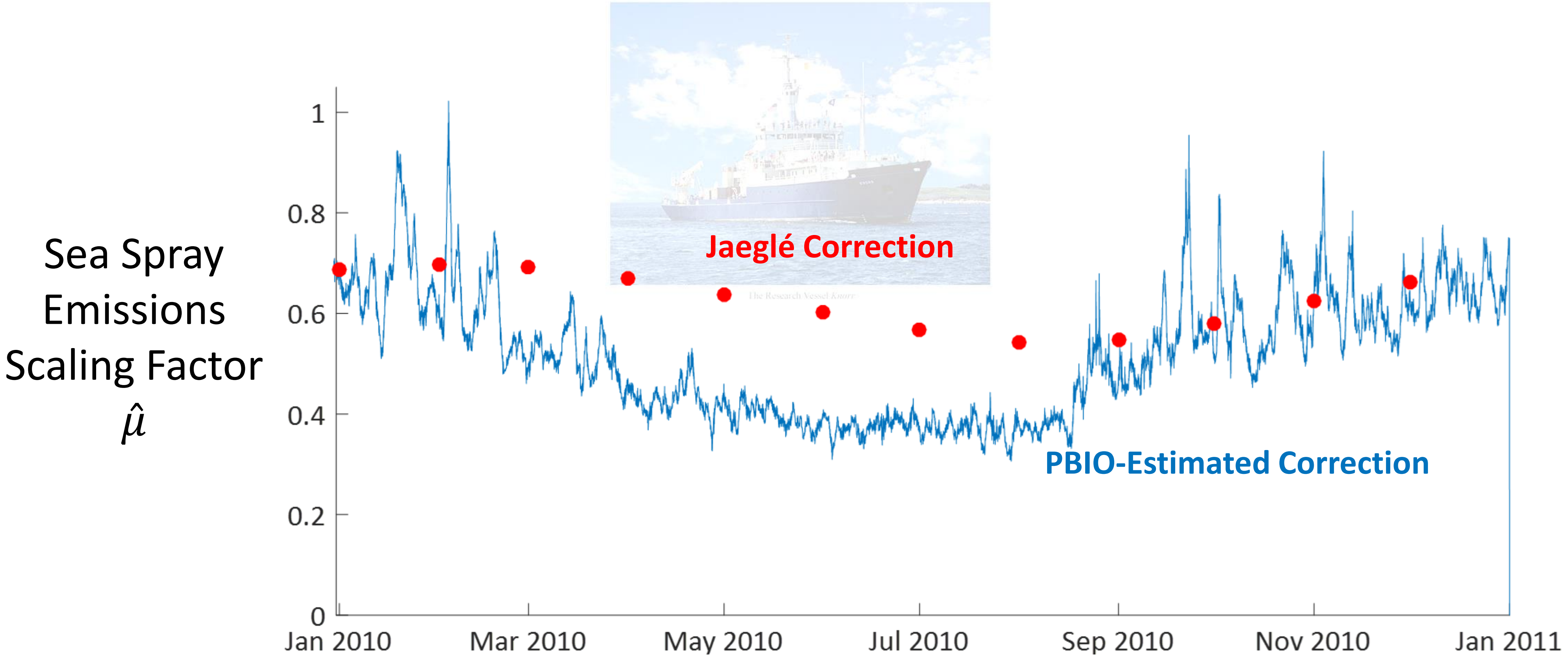
PBIO convergence timescale = 2 hr (inverse gain)





*color bar cutoff (darkest area has value of 5.2 μgm^{-3})

Emission scaling factor trend aligns with sea surface temperature correction in updated model (GEOS-Chem v10-01)



Jaeglé, L. et al. "Global distribution of sea salt aerosols: new constraints from in situ and remote sensing observations". *Atmospheric Chemistry and Physics* (2011)

Summary

- Formulated a passivity-based input observer (PBIO) from process control for atmospheric inverse modeling
  - Can be applied to many other applications, but requires finding ideal inventory variables for unknown input parameters
- Application to sea spray emissions **recovers model update** implemented in later version of chemical transport model
- Estimates of sea spray emission can be improved
  - Improve model prediction of AOD by using **radiative transfer calculations**
  - **Investigate other uncertainties** in sea salt loss terms (e.g. deposition velocity or precipitation fields)
  - Use a combination of other satellite observations for **better data coverage**
- Promising technique for estimating nonlinear aerosol physics with **minimal additional computational effort**

Methods Paper

Sea Spray Paper

Publication DOIs:
Methods - 10.1016/j.compchemeng.2019.06.026, Sea Spray - 10.1016/j.compchemeng.2019.106525

Thank you!

Questions?

Lawrence Livermore National Laboratory

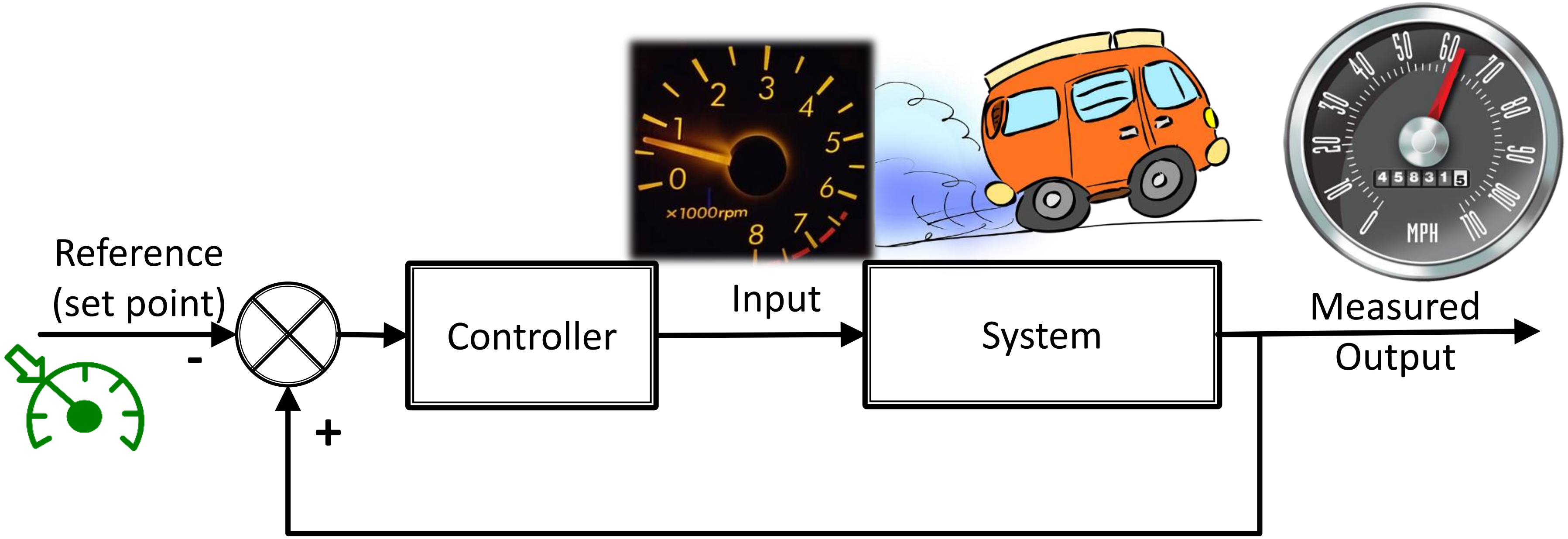
Back up slides

Aerosols affect air quality

Hazardous pollution vs. COVID-19 lockdowns in New Delhi, India

https://www.cnn.com/2020/03/31/asia/coronavirus-lockdown-impact-pollution-india-intl-hnk/index.html

Input Observers are online estimation tools



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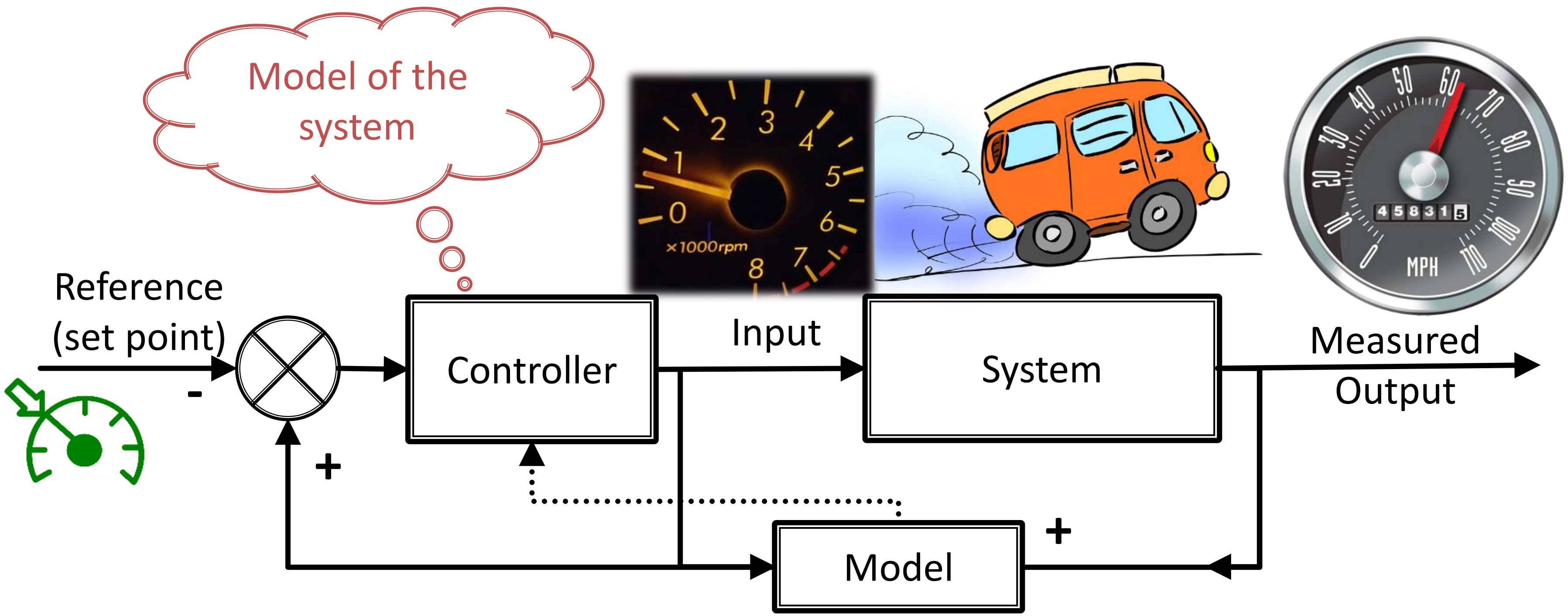
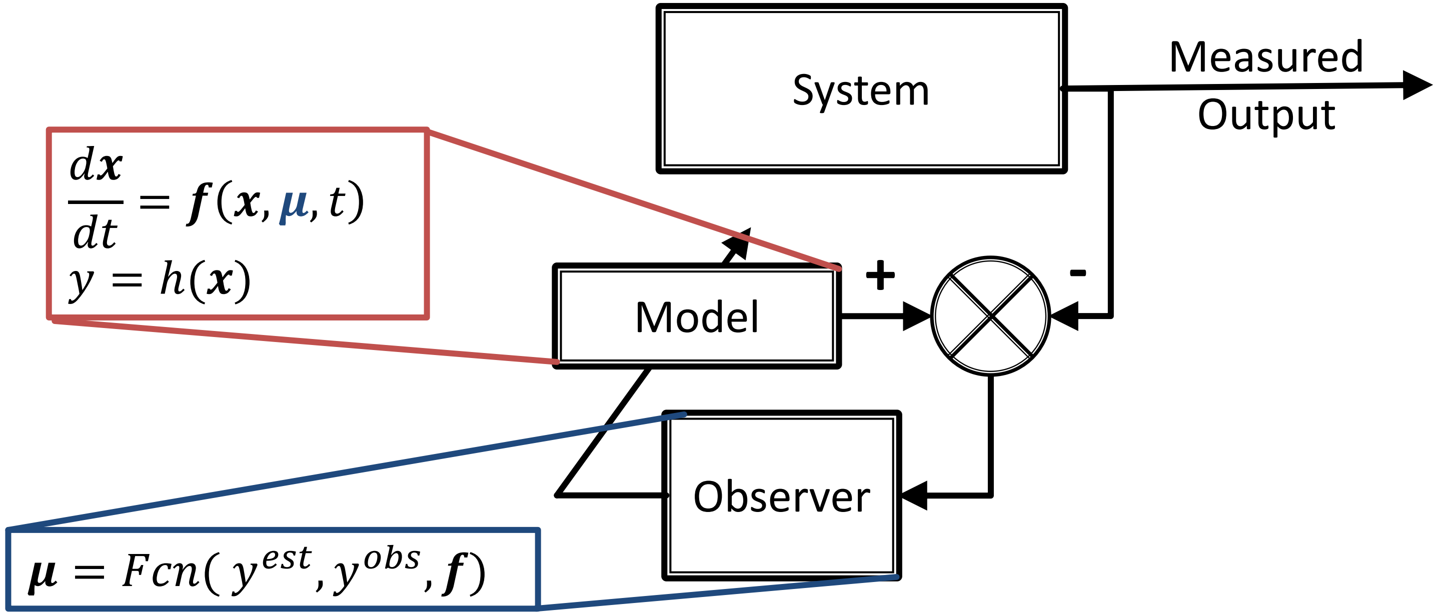
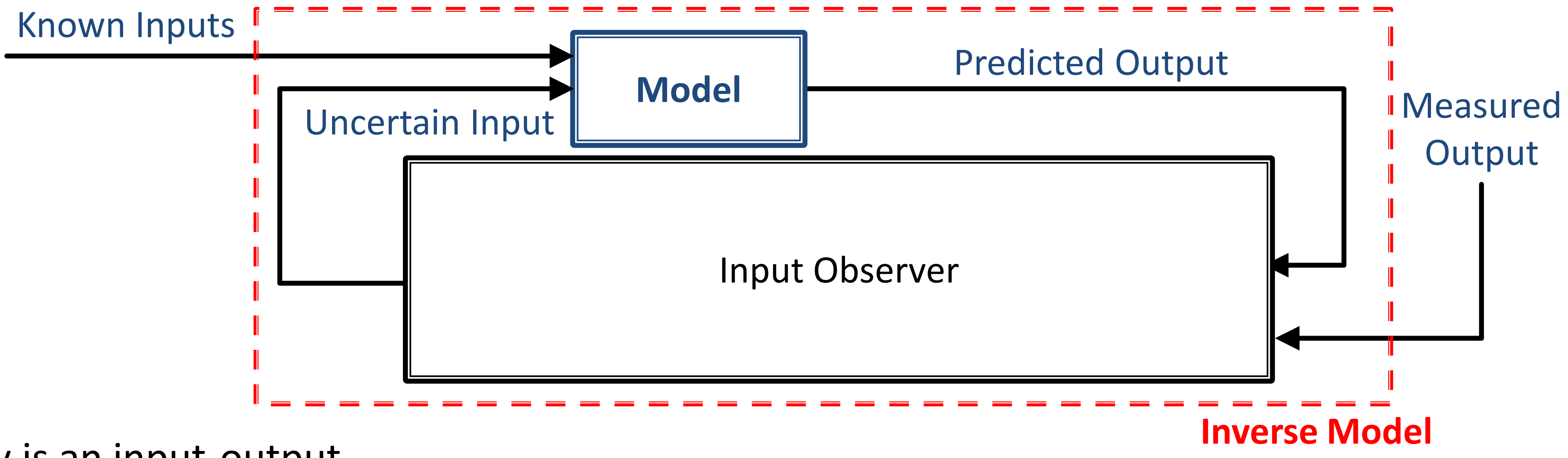


Input Observers are online estimation tools

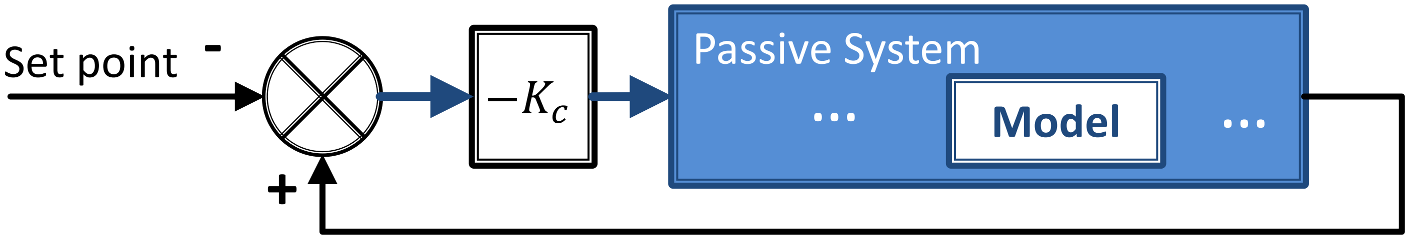
$x(t)$: differential variables
μ: input variables/parameters
y: output variables (measureable)



A passivity-based input observer is desirable



- Passivity is an input-output property
- Proportional feedback to any passive system results in a stable system!

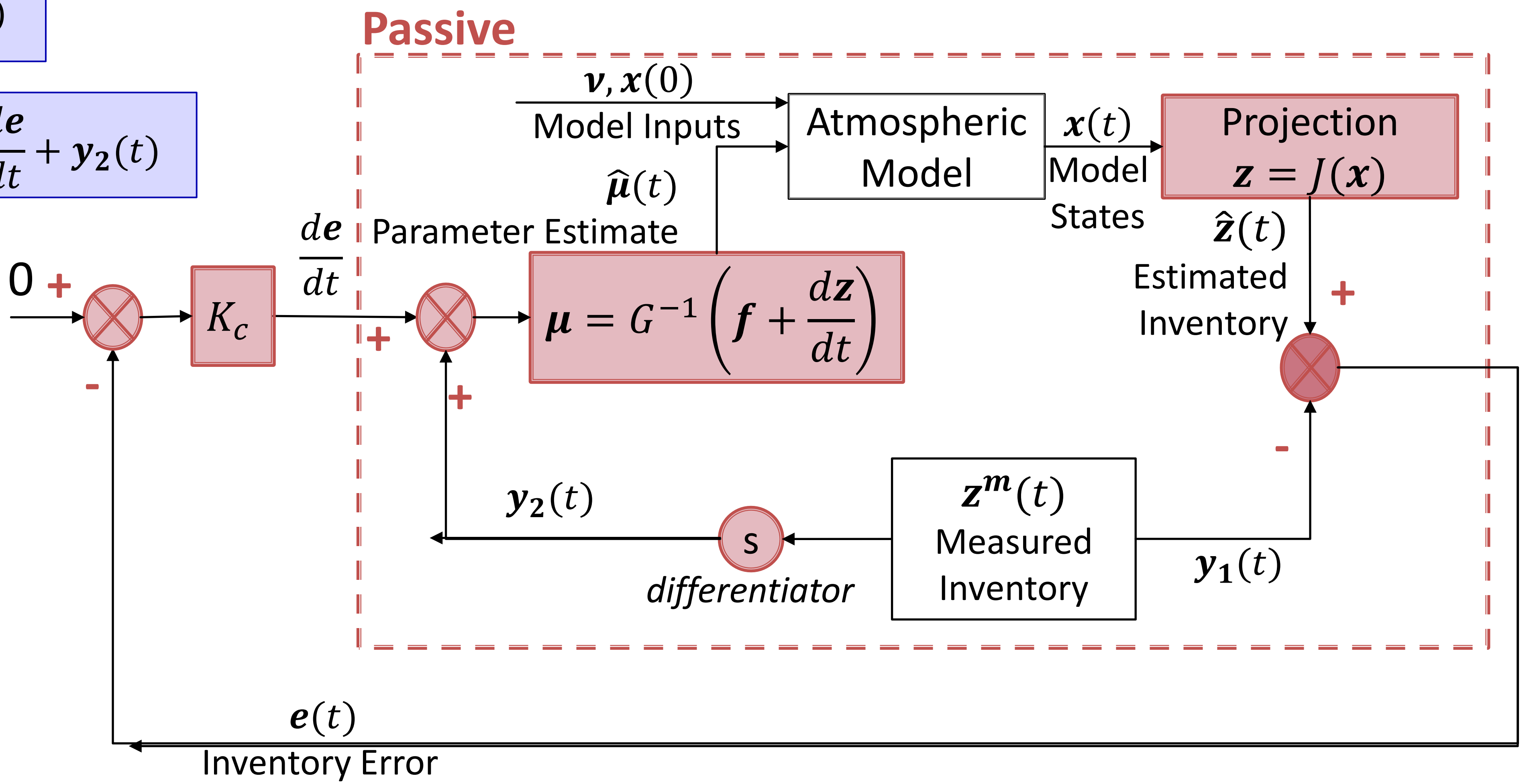


Passivity-based input observer applies proportional feedback to the passive system's output

PBIO block diagram

$$\frac{d\boldsymbol{e}}{dt} = -K_c \boldsymbol{e}(t)$$

$$\frac{d\hat{\boldsymbol{z}}}{dt} = \frac{d\boldsymbol{e}}{dt} + \boldsymbol{y_2}(t)$$



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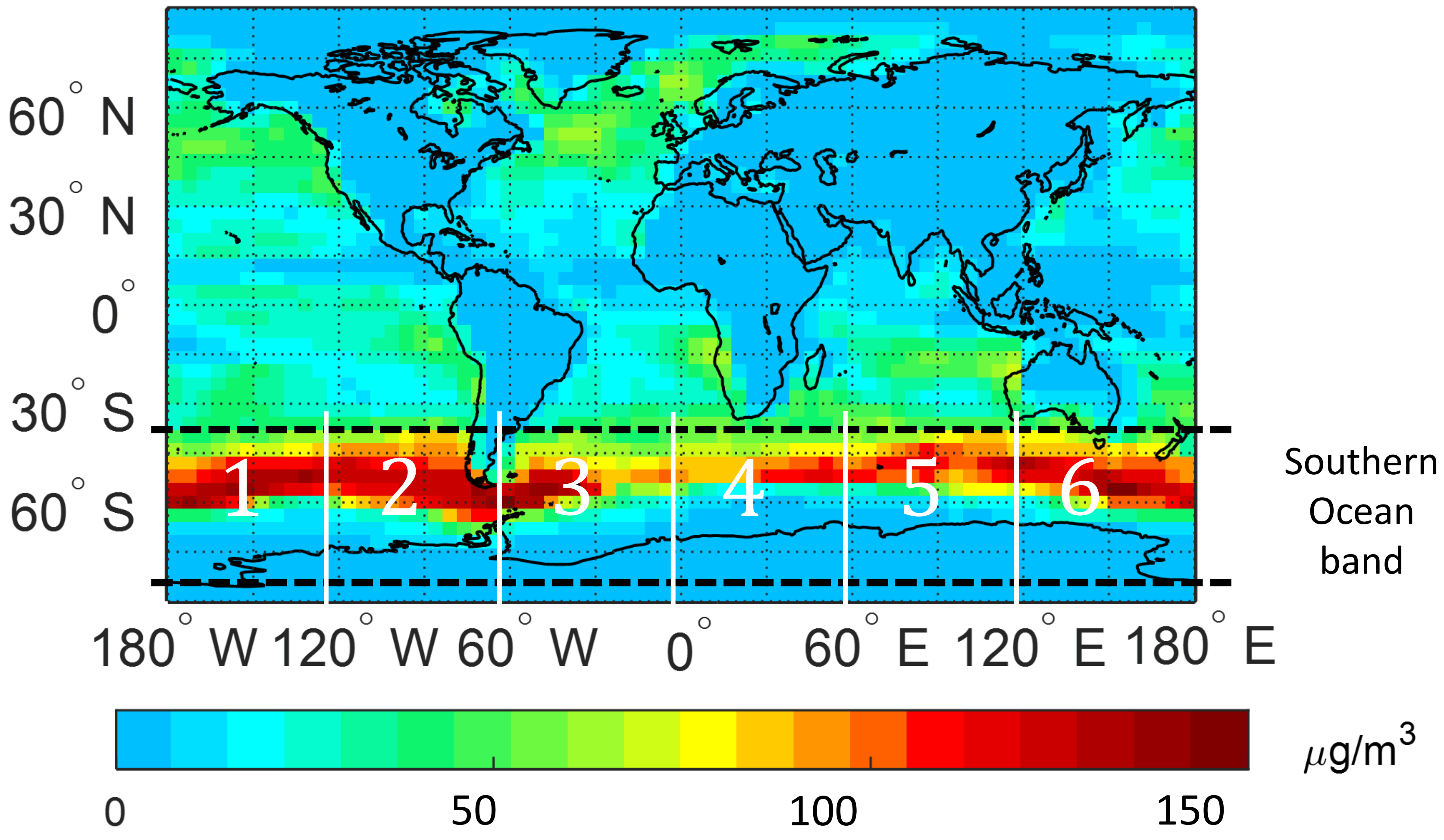
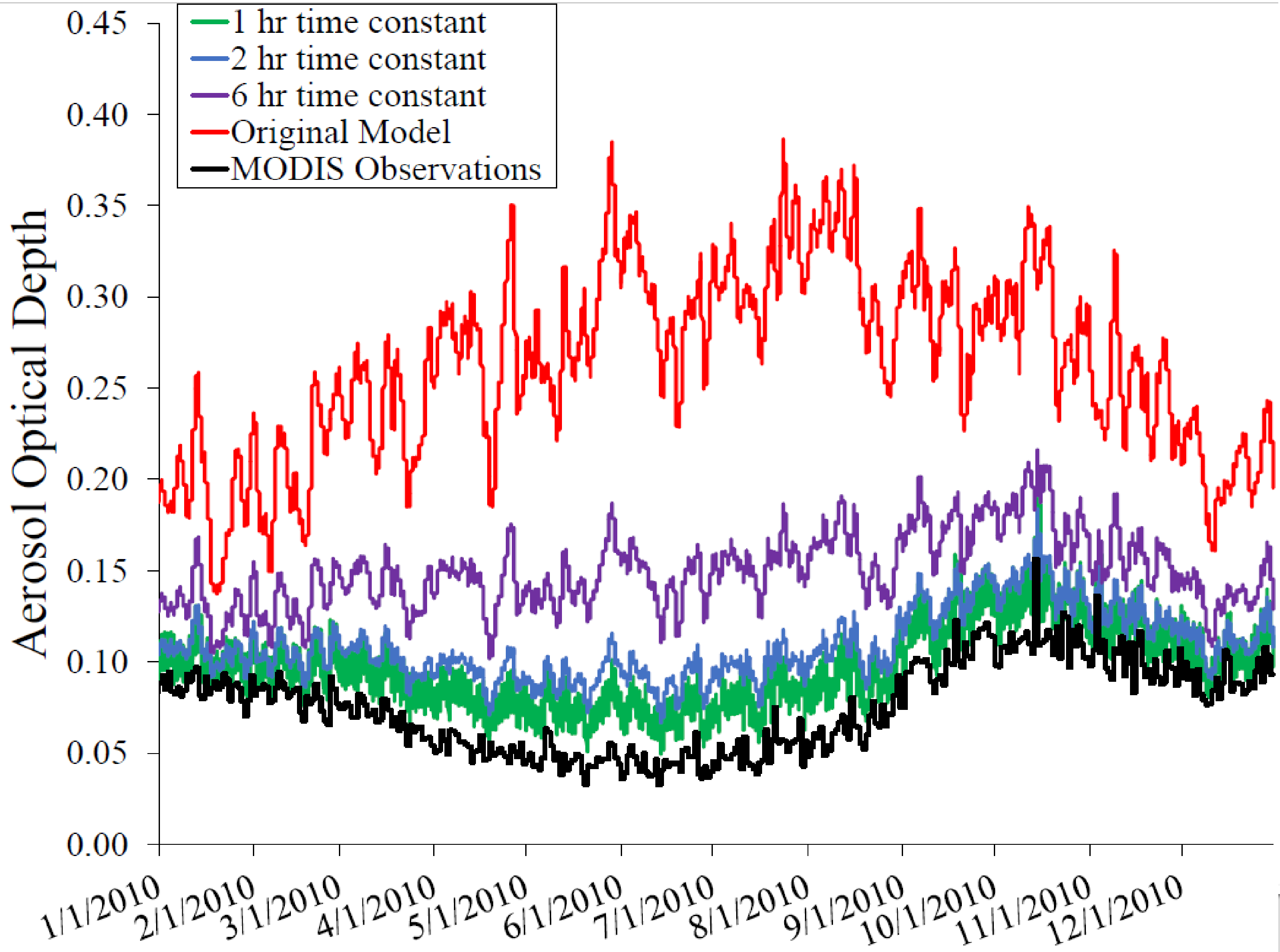
Global model over-predicts sea salt concentration over the Southern Ocean band

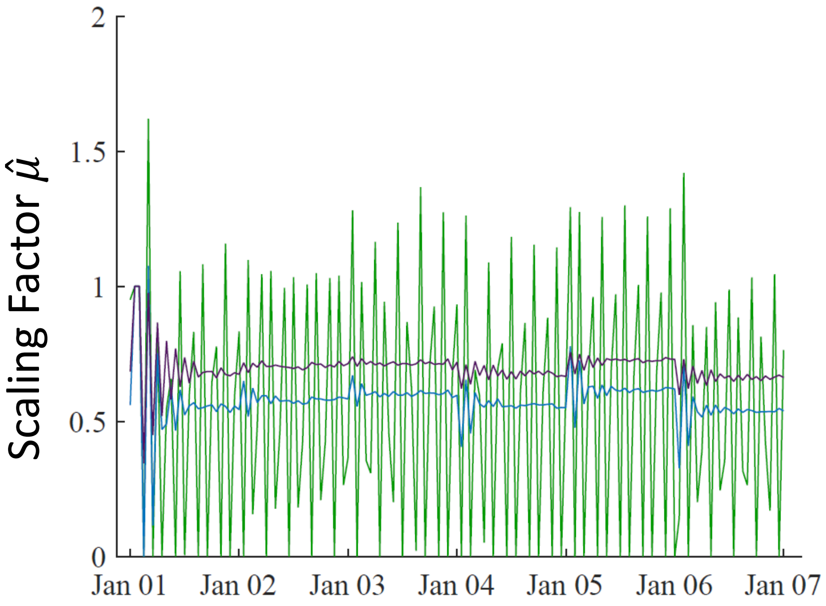
- October 2010: Surface NaCl aerosol concentration
- Predicted by GEOS-Chem TOMAS v9-02 at 4°x5° horizontal resolution
- 6 estimators distributed throughout Southern Ocean band



PBIO Tuning



1 hr time constant
2 hr time constant
6 hr time constant
Original Model
MODIS Observations
Aerosol Optical Depth
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1/1/2010
2/1/2010
3/1/2010
4/1/2010
5/1/2010
6/1/2010
7/1/2010
8/1/2010
9/1/2010
10/1/2010
11/1/2010
12/1/2010



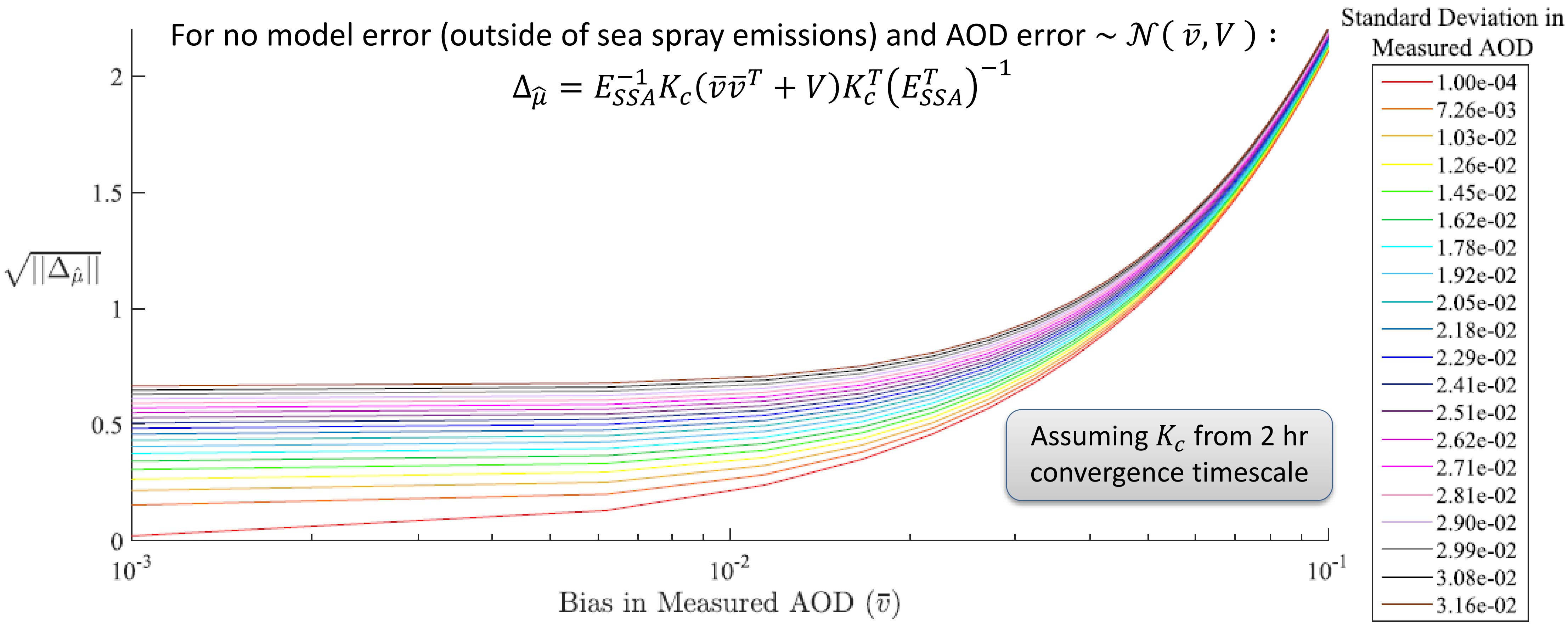
Scaling Factor $\hat{\mu}$
2
1.5
1
0.5
0
Jan 01
Jan 02
Jan 03
Jan 04
Jan 05
Jan 06
Jan 07

Scaling factor uncertainty depends on measured AOD variance and bias

Scaling factor mean-squared error : $\Delta_{\hat{\mu}}$

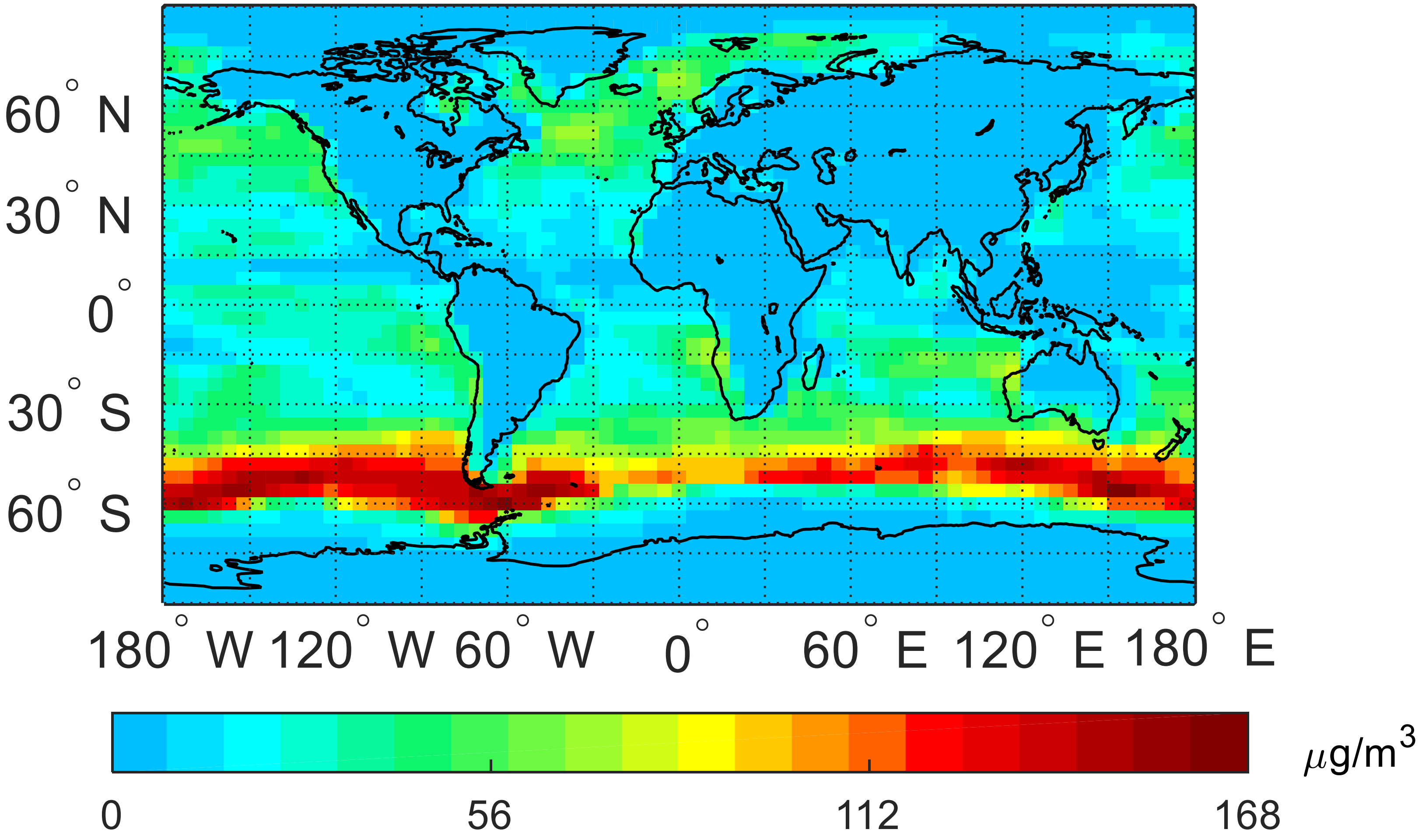
For no model error (outside of sea spray emissions) and AOD error $\sim \mathcal{N}(\bar{v}, V)$:

$$\Delta_{\hat{\mu}} = E_{SSA}^{-1} K_c (\bar{v}\bar{v}^T + V) K_c^T \left(E_{SSA}^T\right)^{-1}$$



Assuming K_c from 2 hr convergence timescale

Original GEOS-Chem Predicted Sea Salt Aerosol at Surface



Estimated Sea Salt Aerosol at Surface